Ph. D. SYNOPSIS

On

Simulation of Lead Free $CH_3NH_3SnBr_3$ PSC with HTL NiO_3, by SCAPS-1D

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2024

Introduction:

This is mainly related to the structure of solar cells and its simulation. The performance as well as efficiency, are going to be studied under SCAPS 1-Di.e. Solar Cell Capacitance Simulator. On earth, we have limited and non-renewable resources of energy to consume, like- petroleum products. We just have solar energy, which is endless and unlimited to use. For this, we need to convert the solar energy to the desired energy form. These devices are called solar cell.

Solar Cell: These are also called photovoltaic cells, which convert energy of light into electrical energy directly. Their electrical characteristics, such as voltage, resistance, current etc., change or vary according to exposure of light. A single solar cell produces 0.5V-0.6V. of current. A combination of these solar unit is called solar panel.

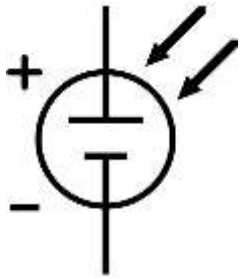


Fig. Symbol of solar cell

We have mainly three types of materials – metals, non-metals and semi-conductors. For solar cell formation, we use semiconductors like silicon.in silicon, every atom has a covalent bond with another and is tetravalent in nature. To make a solar cell work, we need to add impurities to, it which is called doping. There are two type of doping: trivalent impurities and penta-valent impurities.

Trivalent; - p-type, holes majority charge, electrons minority charge, boron, gallium, aluminum, etc. Pentavalent; -n-type, electrons majority charge, holes minority charge carrier, arsenic, phosphorus, germanium, etc.

When p and n type materials combine, the layer in between is called the depletion layer, where no mobile charge is present, It act as a barrier that controls the electron and hole flow through the path. This is the main part of a cell upon which a solar cell works.

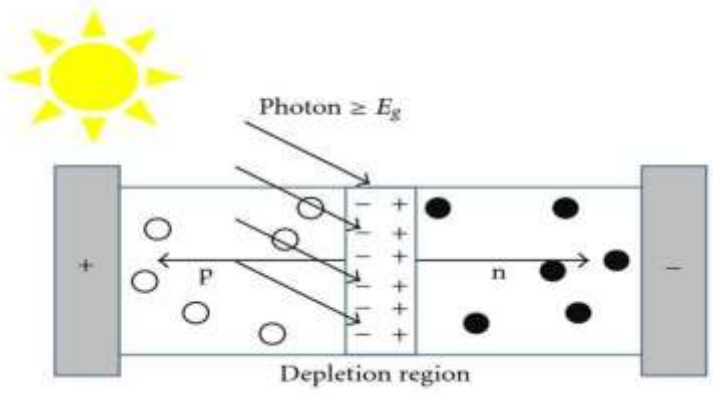


Fig : Photovoltaic Effect

In a solar cell, the main is the photovoltaic effect. Photons, or light, fall upon the n-region with light energy E=hv. Photons pass through the n-type layer and strike to the depletion layer and holes as well as electons of the depletion layer get free and excited, which in turn results into electric flow. This is called generated electromotive force and current the flowing is called photocurrent.Before that, we show know the following key words that we are going to use in the study :

Fill Factor = define the quality of a solar cell.More of the Fill Factor, the better the cell quality

$$\boldsymbol{FF = P_{max} / I_{sc} \times V_{OC}}$$

Fill factor for cells lies between 0.8 to 0.9, mostly

Maximum power = maximum current × maximum voltage

Open circuit voltage (V_{OC}) = Is the maximum amount of voltage when no current is flowing through a circuit.It depends upon cell technology and cell temparature.It is always greater than the maximum volatge.

Current density = Electric current per cross-section area

Absorbtion cofficient =Probability of absorbtion of photons per unit length to the total transitions.

Short circuit current (I_{SC}) = $I_{SC} > I_m$

When there is no voltage drop cross the circuit is called short circuit current.Depends upon cell technology, area of a cell and the solar energy amount provided. It is always greater than maximum current

PCE = power conversion efficiency: output energy per second to the incident light energy per second. PCE = P_{max} / P_{input}

Defect Density= Number of defects detected per lines . Lower the defect density better the software quality.

J_{SC} = cell short circuit current or Maximum current that flows through a solar cell when voltage across the circuit is zero.

Recombination = when electrons in conduction band surpasses the energy gap and reache the valance band and become stable by occupying the holes position , in the valance band.

Literature review: In 1958, Calvin developed the first organic solar cell on magnesium phthalocyanine (MgPc) achieved 200 Mv [22].The first chalcopyrite solar cell, were developed in 1970 based on Ga-Free absorbers. After 1990s, significant improvements were seen by alloying of Ga into the compound.

A three stage, processer was invented in 1994 and appreciated in the fabrication of CIGS devices [6]. In 2000, a study found that thin-film solar cells had a quite complex electronic structure, like glass, MO, two layer of CIGS. A structure layer of CuIn3Se/Cd buffer/ two-layer of ZnO, window [1]. The basic equation to understand the mechanism is poison equation [1].

By 2009, solar cells had attracted very high attention because of their unique properties, like high efficiency, easy solution process for low-cost fabrication. [4] In 2010, research was held for efficiency enhancement in organic photovoltaic cell to optimize series resistance. Photovoltaic cells are a viable option for a sustainable and better future to us, but it is necessary to increase the basic factors of an electrical parameter of a cell. Thin film solar cells are a good alternative to silicon technology because of their J-V characteristic, absorber layer and buffer layer thickness, short circuit current, defect density, open circuit voltage, fil factor structure and efficiency. But optimized solar cell efficiency is > 22% under AM 1.5G spectrum [10]. In 2013, Johan Lindahl, Uwe Zimmermann el.at. carried out a simulation on the solar cell, co-evaporation of high efficiency solar cell and module in depth grading of Ga was successful to enhance efficiency in Cu(InGa)Se_2(CIGS) based cell [7]. The highest efficiency for labs was 20.3% for solar cell [8] Installation of photovoltaic module has increased rapidly over the decades. World-wide only about 2% electricity is produced by solar cells.

Special material such as organic and inorganic metal halide-perovskite materials highly and effectively absorber materials that can be used for the next generation [18]. Next generation does not mean by any year of invention, but because of the used materials arrangement in cell construction.[23]. Perovskite solar cells have three-dimension crystallographic structure with stoichiometry of ABX_3[30].

A- Organic cation

-methyl-ammonium

B - Inorganic

- cesium (Cs)

- Rubidium (Rb)

X – Halide anion

-Iodine (I)

-Bromine (Br)

By using SnS layer between back electrode and absorber layer which will work electron blocking hole transport layer; the efficiency of solar cell gets increased by 14.67% [20] Using TiO_2 at the place of CdS as CdS buffer layer is toxic and it cause optical loss in visible range.[20]. Efficiency of ETL was calculated as 15.71%. TiO_2 was also used in a study in2019 as ETL. By varying its doping level and thickness $CH_3NH_3PbI_3$ difference performance were noticed and efficiency was 30.14% [14] Most important factor is tunneling of electrons. In 2007 J.Verschragen had conducted a research at SCAPS-1D named as Numerical modeling of intra-band tunneling for hetero-junction solar cell in SCAPS-1D.[3].Intra-band tunneling can increase the current through interface based on WKB Approximation .The model was Cu-IN-S on CU-tape solar cell Simulation was performed without and with intra-band tunneling and current transport properties.[3].He concluded that CuI/$CuInS_2$ interface has no restraint on the light current, we can say thus no limitation on solar cell efficiency.[3].

An orthogonal structure of CZTSNPs is used as a hole transport layer in PSC, its efficiency was about 13.41% as it can easily extract holes out of PVSC [11] It has good property of opto-electrical so it can be a better option for the future to use in a large scale at industries [11]

In 2018, the novel technique of MIS-CELIV was performed to calculate electron-hole mobilities.It was mainly focused on complete blocking of one type of charge carrier, with use of suitable insulator [13] It was performed to model organic solar cell efficiency. Concluded that photo-carrier generation efficiency associated with charge carrier mobility of organic solar cell [13].

By Ateeq UL Rehman and coresearchers in 2024,a lead free solar cell was constructed by using $FASnI_3$ is non-toxic.They finally observed that by perfecting the acceptor density and thickness of hole transport layer in a solar cell we can effectively improve the efficiency. But temperature increment would be favorable to the performance [35] When thickness of absorber layer is

increased short circuit current J_{SC} increased. When 100nm to 900nm 7.19% to 13.85% but if increased more like 900nm to 1500 nm.it get reduced as 13.85% to 13.64% [21]so we can say that with increasing thickness, photon absorption increases and generation rate, get boosted but when it is increased beyond limits recombination rate get increased and the solar cell performance decreased [21] Nominal operating temperature should be 43°C but the solar cells have more effective performance at increased or elevated temperature [16]

Doing fabrication or we can say by a doping hetero structure visible improvement in PCE (power conversion efficiency) with highest value of 14.76% because of charge extraction rate improvement.[33].

Device performance can be improved by reducing the defect density of an absorber layer. As power conversion efficiency and carrier life time are strongly related to defect density [12]. Solutions based deposition technique and low temperature provides us cost-effectiveness and heterostructure cell designing [33]. Material property as well as architecture directly influence device performance [12], by improving metal electrode framing for the active area device performance can be increased. Perovskite solar cell (PSC) research is performed in two phases, simulation and experimental. Perovskite solar cell can compete with photovoltaic technologies for most of the studies we are discussing about simulation software technology but it may not fully resemble to the operational condition, day night cycle, temperature, testing outdoor and weather conditions perfectly. Perovskite based tandem solar cell can convert light more efficiently, then their standalone sub-cells. Electrical parameter like recombination should be studied carefully. Recombination. Recombination rate effects device performance as it increases, charge carrier life time decreases and performance get decreased [25] Recombination is termed in the form of continuity equation form which makes the problem non-linear [2] It has three types mainly in mechanism- radiative effect, auger effect and Shockley-read-hall (SRH) [23].

Radiative recombination – It involves conduction band electrons and valance band hole thus photon get emitted at the bandgap zone. This is dominant in PVSC.

Auger recombination-Transporting released photons to another charge carrier like hole or electron.

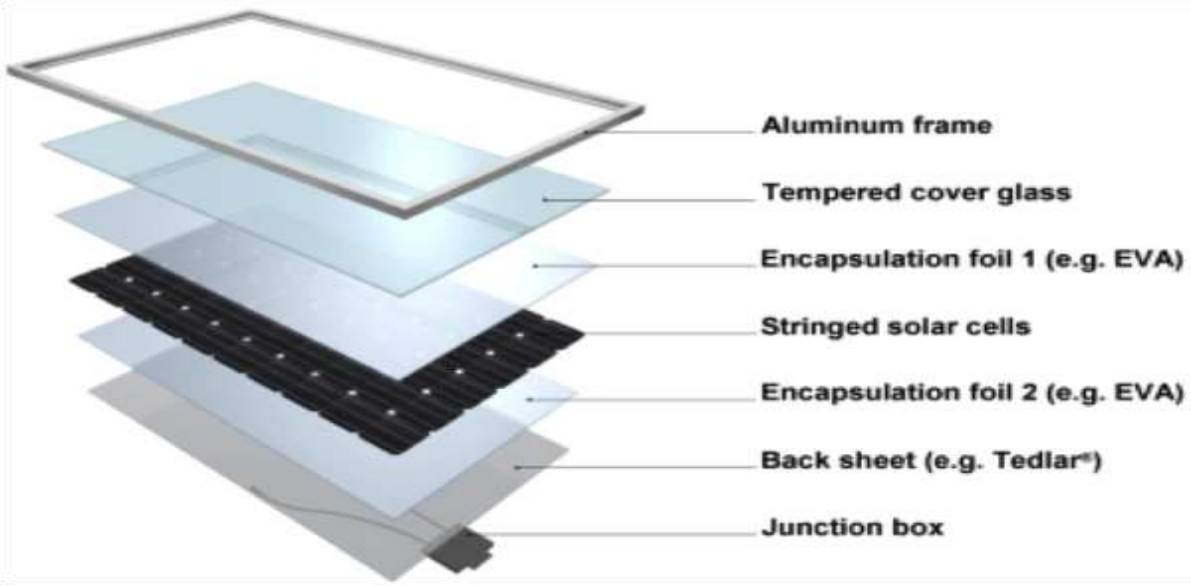
SRH -When charge capturing in the structural defect and traps present in bandgap.[23]

Other two main factors are ETL (electron transport layer) and HTL (hole transport layer) plays an important role solar cell performance [22] A study in2019 by Raoui et. al. was done to compare electron transport layer of ZnO, SnO_2, TiO_2 and some other materials, then calculated that SnO_2 has the efficiency up to 23.55% [23]. When electron transport layer thickness is increased from 10nm to 200nm, the efficiency and fill factor was good up to 40nm with reading 28.04% and o.85, but after that it decreased slowly due to the series resistance increment [19]. when thickness is 150nm -160nm V_{OC} and J_{SC} remain same and beyond 160nm and more V_{oc} and J_{sc} get decreased 0.88v and then zero [19].

Efficiency can also be improved by adjusting parameters like mobility and band gap of solar cell [4] Efficiency loss can arise from cell resistance (R_s) but as a minor factor.This resistivity loss can be reduced by anode conductivity [5] Using SnS as HTL and TiO_2 as ETL efficiency of 27%can be reached.[20]. A back contact material having work function 5.2eV is required for a maximum work performance range.[20]

By doping some special nano-particles we can try to improve solar-thermal properties and absorption improvements [26]. Perovskite solar cells that contain an alloy-based tin and lead have 30% or above power conversion efficiency in single junction solar cell theoretically.[29]. Hussein Sabbah approached a lead-free $CS_2AgBiBr_6$ double perovskite solar cell having p-i-n inverted structure. It has reduced toxicity and improved stability with power conversion efficiency of 6.37[36].

SOLAR PANEL



1. **Aluminum Frame:** It is a perovskite layer provides both mechanical protection as well as an electrical insulator. It is one of the rare-most layer in solar cell.
2. **Tempered Glass Cover:** The outer most layer of a panel should be shiny and unbreakable. It protect the solar panel from dirt dust and harsh weather condition. Its recommended thickness is 3mm-4mm.
3. **Encapsulation Foil: EVA-**Ethylene Vinyl Acetate-is a transparent plastic layer where cells are encapsulated. By EVA a laminated layer is provided on top of cells which holds them together. For extreme temperature and humidity, it should be durable.
4. **Back Sheet:** It is a perovskite layer provides both mechanical protection as well as electrical insulation. It is one of the rare-most layer in solar cell.
5. **Junction Box:** It is a connector between the solar cell module and solar charge controls device.it connects the power generated to external device.

6. **Stinged Solar Cell:** Where thousands of cells arranged together to form a panel called solar panel. Cost and efficiency, decides the overall performance of a solar decide. The solar cell has three layers-

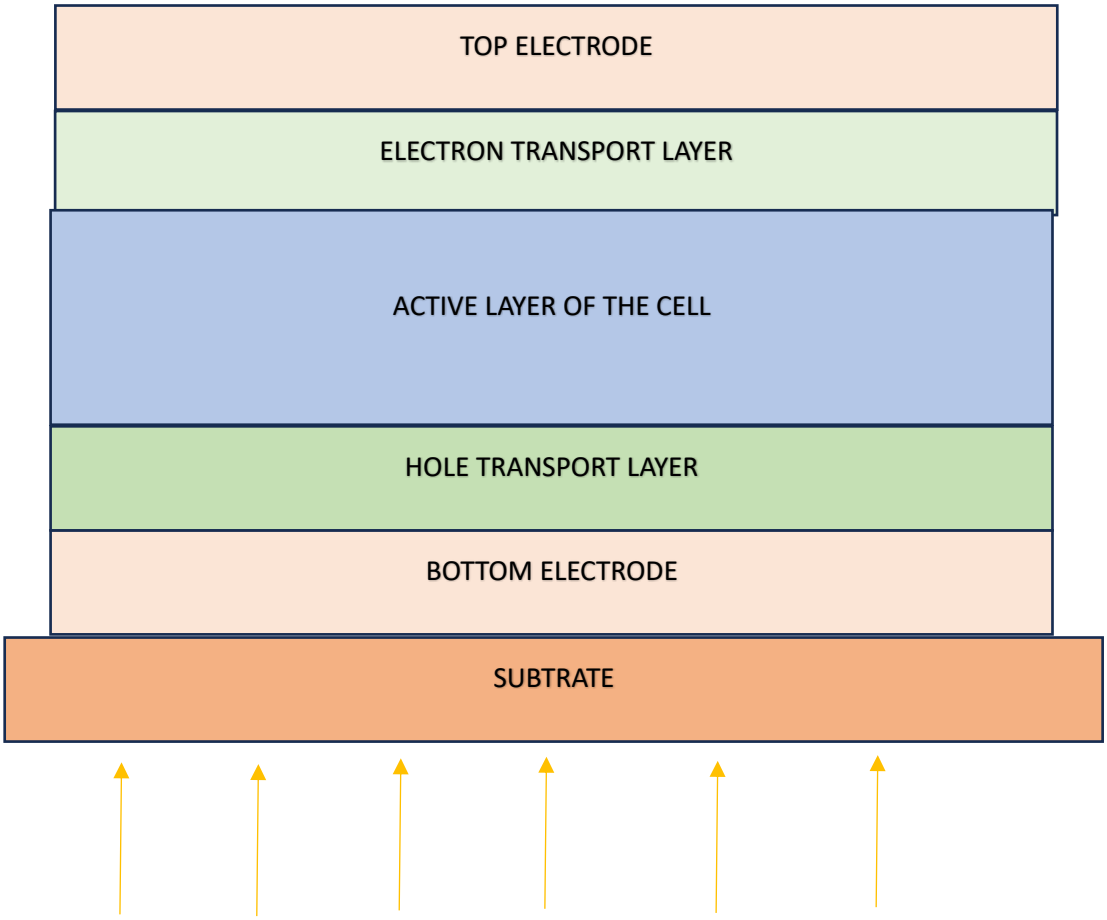


Fig. Solar cell layer

Top layer -n- type, thin layer, high electron concentration

In between -p-n junction, a depletion layer

Bottom layer -p-type, thick layer, high hole concentration

Research Gap: These are the problem seen during literature review which has not been appropriately answered. Our objective explains the related idea better and tries to fill the gap in the selected area of research. We are trying to identify and rectify research are gaps of this topic. It has never been so easy to fill up the gaps of research area.

Some of materials over here are not environment friendly like lead and cadmium. Some has problem of limited source. Others like CdS type material has challenge of optical loss in visible region. Defect density is not very much explained. Some materials get-heat up during processing which should be over-come.

Here we are going to eliminate research gap in the area of solar cell and its structure. Many papers and journals have published but there is no end of research gap. Here we are trying to identify the gaps related to manufacturing and materials used in solar cell. Along with varying parameters of the material used.

Purpose of study–why we need a solar cell which is lead free

1. Toxic
2. Harmful for environment
3. Higher cost
4. Limited source of material
5. Optical loss in visible region

To replace lead based solar cell by organic solar cell with more efficiency and less cost. By SCAPS 1-D we simulated 5 layer of a solar cell which comprises electron-transport layer, hole-transport layer, a perovskite layer, back contact surface and front contact etc. with various changing parameters.$CH_3NH_3SnBr_3$ means bromine-based perovskite is to be fabricated using TiO_2, as a layer of ETL because it provides better electron transfer and long-time stability discussed in earlier studies. As hole transport layer NiO_3 is selected as it

provides better efficiency. FTO fluorine doped tin oxide is to be used as a transport electrode. Direct excitation with light is to be performed in software. By changing temperature, doping density, doping material, material thickness all the changes are to be noted carefully. Curves and graphs are then should be saved. With SCAPS 1-D we will simulate the discussed layers, but some materials, and parameters can vary as per requirement of experiment.

Objective of the study:

1. To manufacture a lead-free solar cell and explaining why we need this type of solar cell in future
2. To enhance its fill factor by controlling electron and hole tunneling effect
3. To study the importance and impact of material thickness on solar cell performance.
4. To check defect density of used material and its effect on working of our cell
5. To study the recombination effect and its impact on quality of solar cell

Proposed Research Design and Methodology Adopted: we will use software SCAPS 1-D for simulation.An ideal thin film solar cell program must allow atleast six layers for simulation[2]Tunneling, heat flow, optics like features should be included in a highly developed program.On a thin film when we perform simulation spectral: response,J-V characteristics,capacitance measumement of C-V and C-f ,kelvin probe,SPV surface photo-voltage ,transient measurement of current, voltage and capacitance .[2].tunneling is basically described as a quantum-mechanical phenomenon.[3]. By schrodinger equation ,results in electrone wave vector then we calculate tunneling probability of an electron.[3]The software which we are going to use is the Solar Cell Capacitance structure (SCAPS-1D) for analysis of the solar cell. SCAPS is a software for 1-D solar cell simulation. This software is developed at

ELIS, University of Gent, Belgium under Dr Marc Burgelman. This is freely available to the PV research community.

- Run SCAPS
- Define problem, material and its property
- Specify the situation and define the working points
- Define the required calculation or problem to be simulated
- Start calculations

  Calculations, graphs and curves are displayed.

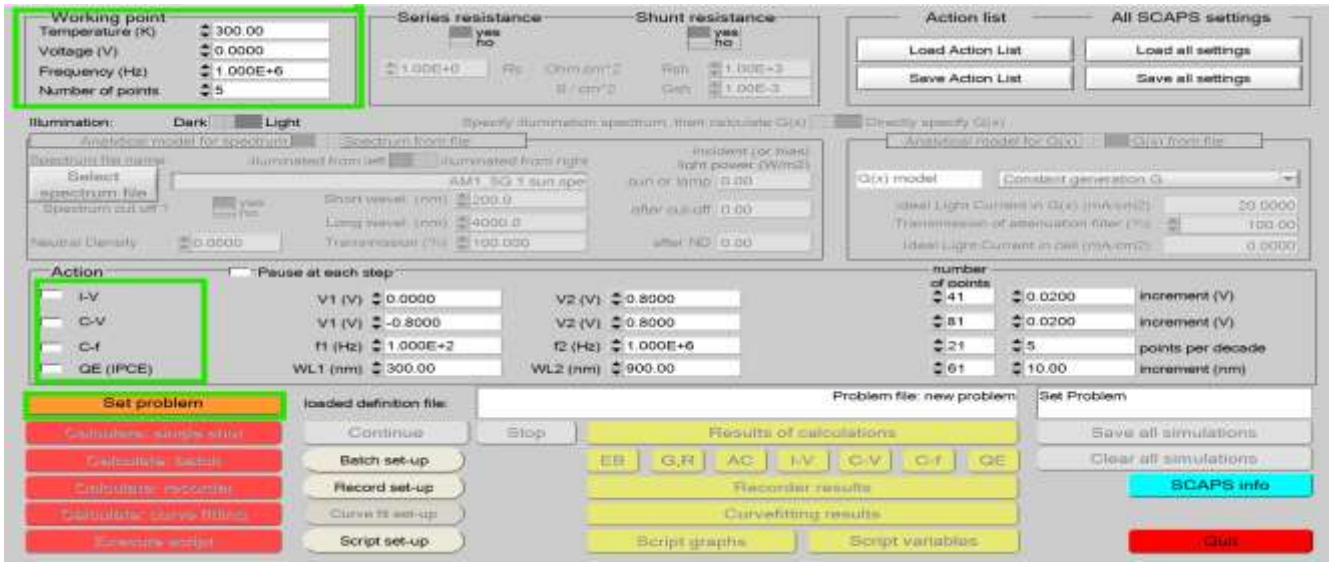


Fig: SCAPS 1-D Start Up

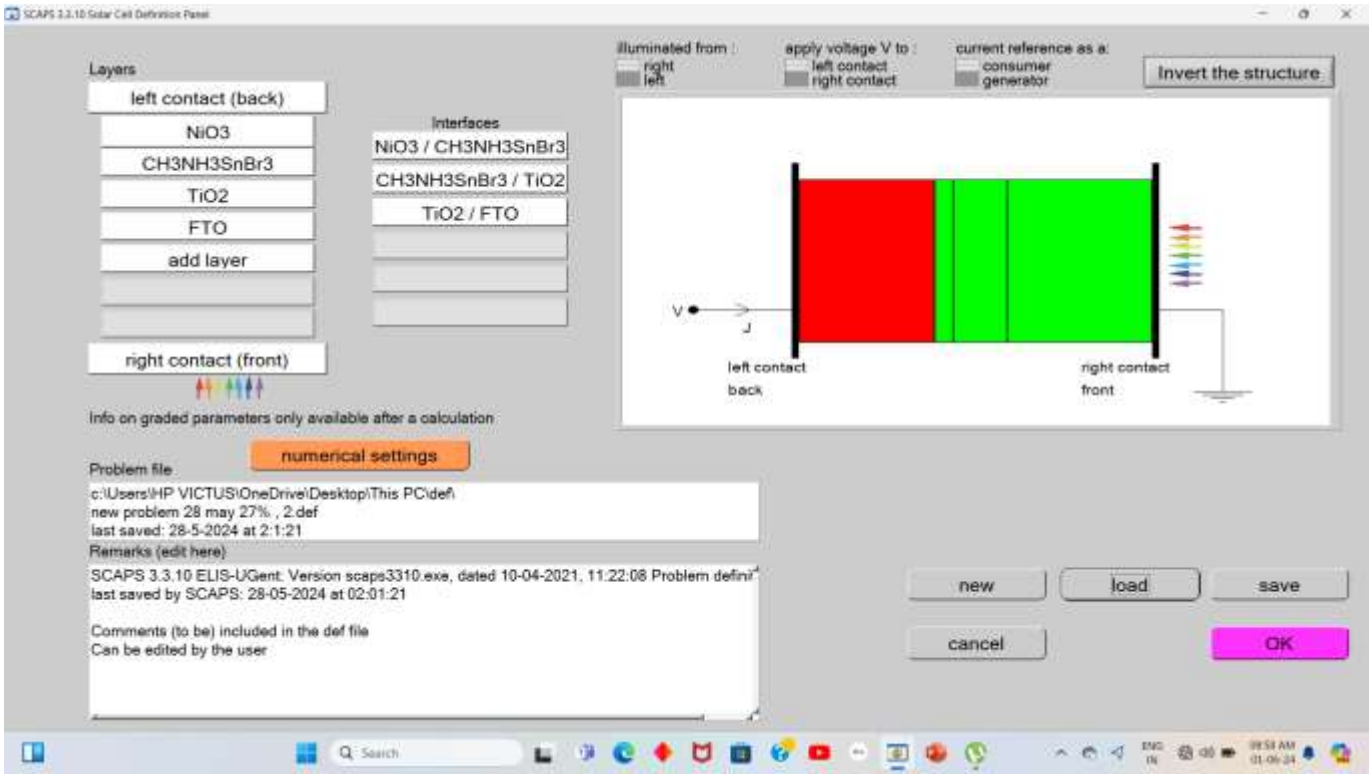


Fig. Material to be used in simulation

To meet future requirements and better opportunities it is required to execute more experiments and research actions.We can perform it by using software as well as practically.

Expected outcome: This synopsis can explain how to manufacture solar cell layers with different materials like metals , semiconductors halides etc.How to arrange every layer of this cell with varying parameters for better performance.Quality of the solar can be characterised by its fill factor, conversion efficiency, short circuit current, open circuit voltage etc.

In the manufacturing and simulation of solar cell,we are going to improve its most of the parameters, to improve the performance of cell.we will try to style it environment friendly but with better properties means more efficiency.

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